

Tennessee State University College of Engineering and Technology Department of Mechanical Engineering

The Impact of Modeling, Simulation, and Characterization of the Mechanical Properties of Nano-materials in the Nanotechnology Industry

> by Dr. Landon Onyebueke

The 2nd U.S. – Korea Forum on Nanotechnology Los Angeles, CA. February 17-18, 2005.

Organization of Presentation

- Introduction
- Goals and Objectives
- Hardware and Software Components
 Research Procedure and Test Results
 Structural Design, Modeling and Simulation
 - Conclusion
- Acknowledgements

Introduction

The development of NEMS and MEMS are critical to the U.S. economy and society because nano- and microtechnologies will lead to major breakthroughs in:
 Information technology and computers
 Medicine and health
 Manufacturing and transportation
 Power and energy systems

5. Avionics and national security

Research Goal and Objective

> To provide a computational modeling Techniques using quantum mechanics, classical atomistic methods, and/or mesoscale simulation to enable scientists to visualize and predict behavior emerging at length scales of up to 100nm. >To provide a non-destructive, rapid, inexpensive procedure for characterizing very thin materials, MEMS, coatings, biomaterials and the emerging nanostuctured materials.

Research Goal and Objective Cont'd

 Mapping variations in mechanical properties of Fused quartz, Copper and aluminum at various depth near the surface to their bulk properties.

Show the trend of mechanical properties changes at the surface @ temperature as high as 500°C



Hardware and Software Components

Nanoindentation for the Mechanical Characterization of Materials Using Nanotest 550

Research Design

>Nanoindentation refers to depth-sensing indentation testing in the sub-micrometer range and has been made possible by the development of ;

*machines that can make such tiny indentations while recording load and displacement with very high accuracy and precision, and

* analysis models by which the load displacement data can be interpreted to obtain hardness, modulus, and other mechanical properties.

Features less than 100 nm across and thin films less than 5 nm thick can be evaluated at forces in the range of 5 to 200mN



NANOTEST 550 EQUIPMENT





Nanotest 550



Nanoindentation Theory

 \geq Application of controlled load to a surface, which causes local surface deformation **Calculates H and E from indentation area** \geq In contrast to AFM, can provide perfectly normal force >Two-plate capacitor detects displacement and electrostatic voltage for force actuation. Sealed chamber – vibration isolation table



NanoTest 550 FEATURES

Mechanical property measurements of materials, thin film and surface layers less than 50nm thick. Depth resolution better than 0.1nm Applied load up to 500mN. Providing the following data: •Load vs. Depth •Hardness vs. Depth •Elastic modulus •Plastic and elastic work

The NanoTest pendulum



150

The NanoTest measures the movement of the diamond probe in contact with a surface. The resultant displacement of the probe into the surface is monitored. The displacement of the diamond is measured by means of a parallel plate capacitor, one plate of which is attached to the diamond holder and displayed in real time as a function of load.

Original design - University of Lancaster, UK, Newey, Wilkins and Pollock, J Phys E, 1982, pp119-122. Micro Materials formed 1988 by Dr Jim Smith.



-ISU



NanoTest Indentation Result (Window) Example

Selected Filename (C/Lboro/bp150							
2767-	Analysis Besults						
2600-							
2400-	Maximum Depth (nm) 2767.4						
2200-	Maximum Load (mN) 442.13						
2000-							
1800-	Plastic Depth (nm) 2577.7						
	Hardness (GPa) 2.72						
fg 1400- →	Reduced Modulus (GPa) 121.40						
1000							
000-	Elastic Recovery Parameter U.U736						
600-	Contact Compliance (nm/mN) 0.57						
400-	Plastic Work (nJ) 433.65						
200-	Electio Work (n. D. 71.02						
14-	Elastic work (nJ) 71.33						
0.1 50.0 100.0 150.0 200.0 250.0 300.0 350.0 400.0 442.1 Fitting mean square error 3.4012							
Cursor Position Load (mN) 219.98 Depth (nm) 1386.53							
Load Axis (mN) Depth Axis (nm)							
Grid C Auto Scale G Grid C Auto Scale G	Indentation number 5						
Maximum 500.0 Maximum 1000	Load cycle number 1 (<< Previous) (Naxt) (All)						
Mininum 0.0 Mininum 0							

Plots of hardness and Modulus for fused Quartz



Plots of max and Plastic depth with Max load for Fused Quartz



-ISU

250 200 100 100 50 -1 9 19 29 39 Indent #

Max load for indentatiom

Analysis of fused quartz Nanoindentation

Analysis .. Oliver and Pharr Epsilon is .75 using 80% of the unloading curve

Indent	Depth h (nm)		Load	Hardness	Modulus	Work(nJ)	
	Max.	Plastic	Max.(mN)	(GPa)	(GPa)	Plastic	Elastic
1	1132	819	200.34	8.498	73.15	30.3765	48.3311
2	1145	835	200.41	8.183	72.45	30.5079	48.1685
3	1140	829	200.17	8.302	72.31	29.9929	48.1685
4	1136	827	200.34	8.351	72.87	30.1212	47.8873
5	1135	827	200.09	8.33	73.01	30.0401	47.6618
6	1136	824	200.23	8.4	72.87	30.0697	48.1257
7	1137	829	200.12	8.302	72.73	30.3205	47.6567
8	1143	834	200.3	8.211	72.1	30.541	47.6714
9	1139	829	200.28	8.309	72.66	30.3888	47.9033
10	1140	829	200.02	8.281	72.52	30.1538	47.934
Average	1138.3	828.2	200.23	8.3167	72.667	30.25124	47.95083

Test Result Aluminum

Hard. vs Disp. Plot





Other NanoIndentation Study

Mapping variations in hardness and elasticity at the nanoscale

Precise indent placement with a 4-objective high resolution metallurgical microscope

NOTE: 1 objective can be replaced by contact/AC mode SPM



Indentations along 10 µm alloy interface between stainless steel surfaces



studies of nano- and micro- scale phase separation



Nanomechanical property testing at high temperatures

Horizontal loading configuration has advantages for drift-free high temperature tests

Hot stage specifications

- Indentation to 500 degrees
 Celsius
- Scratch testing to 500 degrees
 Celsius
- Thermal drift minimal





Contact fatigue testing

An accelerated test to mimic the mechanical fatigue cycles which circuit boards and ME devices are subject to in service

Information obtained:

1/ time to failure (durability)2/ type of failure (adhesive/cohesive/mixed)



Assess adhesion/delamination (e.g. between metal-dielectric)
Investigate fracture behaviour



- Depth Profiling Determination of hardness and Young modulus variations with depth at a single point
- Creep Time dependent creep and flow behaviour revealed by plots of depth vs. Time at constant force.
- Scratch Testing -- Testing Film adhesion by measuring displacement, friction and acoustic emission during scanning with increasing applied force.
- Small scale Wear testing Change in depth with time during repeated low load scratching over the same area.
- Thin film and coating adhesion _ Steps in Depth vs. Force curves due to cracking and adhesion failure.
- Impact Testing Change in indentation depth with time due to repeated impacts at constant force
- High Temperature testing Mechanical property variation at higher temperatures.

Structural Design, Modeling and Simulation

- Nano- and microelectromechanical systems
- Carbon nanotubes and nanodevices
- Direct-current micromachines
- Induction motors
- Microscale synchronous machines
- Nanoactuators and sensors
- Nanomotors and nanogenerators, etc



Conclusion

- To comprehensively study nano-materials, advanced modeling and computational tools are required primarily for 3D+ data intensive modeling and simulations.
 - Nanoindentation techniques are essential in the optimisation of the mechanical properties of thin films and coatings
- 3. The NanoTest has large range of testing techniques, and therefore offers a complete testing capability
- 4. These techniques are possible due to the unique pendulum design
- 5. The high temperature option and impact module allow testing under contact conditions that can closely simulate those in service

ACKNOWLEDGEMENT

- Most of the work presented in this Forum are taken from:
- Research work sponsored by NASA and Tennessee State University
 Book written by Serey Edward Lyshevski They are gratefully acknowledged for their

contributions to Research in Nanotechnology